# Parallel netCDF: A High Performance API for NetCDF File Access

#### **Overview**

Parallel netCDF (PnetCDF) is a library providing high-performance I/O while still maintaining file-format compatibility with Unidata's NetCDF.

NetCDF gives scientific programmers a space-efficient and portable means for storing data. However, it does so in a serial manner, making it difficult to achieve high I/O performance. By making some small changes to the API specified by NetCDF, we can use MPI-IO and its collective operations.

- <u>Download</u> has the latest release and development links as well as information about svn access.
- Documentation: a QuickTutorial, plus papers, presentations, articles, and other resources
- Benchmarking: tools and suggestions for evaluating pnetcdf performance

#### **News**

- In the 1.3.0 release, the unsigned and 64-bit integer data types are supported for CDF-5 format. The unsigned data types include NC\_UBYTE, NC\_USHORT, NC\_UINT, and NC\_UINT64. The 64-bite integer data types are NC\_INT6 and NC\_UINT64.
- APIs for the new data types are supported. For C, they are ncmpi\_(i)put/(i)get\_var\*\_ushort/uint/longlong/ulonglong. For Fortran, they are nfmpi\_(i)put/(i)get\_var\*\_int8.
- A new set of "buffered"-put APIs is supported in 1.3.0 release. The nonblocking iput/iget APIs require the contents of user buffers not to be changed until the wait call completed. The bput APIs use a user attached buffer to make a copy of request data, so the user buffer is free to change once the bput call returns.
- The special character set, "special2", and multi-byte UTF-8 encoded characters introduced in the CDF-2 file format for variable, dimension, and attribute name strings are now supported.
- A set of example programs and **QuickTutorial** are now available.
- Nonblocking I/O is redesigned in the 1.2.0 release. It defers the I/O requests until "wait" call, so small requests can be aggregated into large ones for better performance.
- Two new hints, nc\_header\_align\_size and nc\_var\_align\_size, are added. The former allows pre-allocation of a larger header size to accommodate new header data in case new variables or attributed are added later. The latter aligns the starting file offsets of non-record variables. Refer to <a href="VariableAlignment">VariableAlignment</a> for a more detailed description.
- Data consistency control has been revised. A more strict consistency can be enforced by using NC\_SHARE mode at the file open/create time. In this mode, the file header is synchronized to the file if its contents have changed. Such file synchronization of calling MPI\_File\_sync() happens in many places, including ncmpi\_enddef(), ncmpi\_redef(), all APIs that change global or variable attributes, dimensions, and number of records.
- As calling MPI\_File\_sync() is very expensive on many file systems, users can choose more relaxed data consistency, i.e. by not using NC\_SHARE. In this case, file header is synchronized among all processes in memories. No MPI\_File\_sync() will be called if header contents have changed.

  MPI\_File\_sync() will only be called when switching data mode, i.e

  ncmpi\_begin\_indep\_data() and ncmpi\_end\_indep\_data().

## A note about Large File Support

As of Pnetcdf-0.9.2, we ship with support for <u>CDF-2</u> formated data. With this format, even 32 bit platforms can create netcdf datasets (files) greater than 2GB in size. See the file README.large\_files in the source tree for more information. CDF-2 also allows more special characters in the name strings of defined dimension, variables, and attributes.

The maintainers of the serial NetCDF library added support for the CDF-2 format in netcdf-3.6.0. The support was based largely on work from Greg Sjaardema.

The <u>CD-5</u> file format specification: supports unsigned and 64-bit integer data types and variables with more than  $2^{32}$  array elements.

The <u>CDF (or CDF-1)</u> file format specification has been in use through netCDF library version 3.5.1.

#### File and Variable Limits

Both PnetCDF and NetCDF share limitations on file and variable sizes. More information can be found on the <u>FileLimits</u> page.

## **Required Software**

PnetCDF requires an MPI implementation with MPI-IO support. Most MPI libraries have this nowadays. A parallel file system would also go a long way towards achieving highest performance.

## **Related Projects**

PnetCDF makes use of several other technologies.

- <u>ROMIO</u>, an implementation of MPI-IO, provides optimized collective and noncontiguous operations. It also provides an abstract interface for a large number of parallel file systems.
- One of those file systems ROMIO supports is <u>PVFS</u>, a high performance parallel filesystem for linux clusters.

Today, there are several options for high level I/O libraries. Here are some discussions on the role of PnetCDF in this ecosystem:

- pnetcdf\_vs\_hdf5?
- pnetcdf vs netcdf4?

#### **Mailing List**

We discuss the design and use of the PnetCDF library on the parallel-netcdf@mcs.anl.gov mailing list. Anyone interested in developing or using parallel-netcdf is encouraged to join. Visit the list information page for details.

The URL for the list archive is <a href="http://lists.mcs.anl.gov/pipermail/parallel-netcdf/">http://lists.mcs.anl.gov/pipermail/parallel-netcdf/</a>. You can broswe even older mailing list messages at the older <a href="mailing-list-archives">mailing-list archives</a>

## **Project Members**

- Rob Latham, Rob Ross, and Rajeev Thakur (Argonne National Lab)
- Wei-keng Liao, Seung Woo Son, and Alok Choudhary (Northwestern University)
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- Jianwei Li (Northwestern, graduated in 2006)
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#### **Citations**

When referring to the Parallel netCDF project, please use our "permanent" URL: www.mcs.anl.gov/parallel-netcdf. The 'trac' or 'www-unix' URLs could change.

If you are looking for a reference to use in a published paper, please cite our SC2003 paper

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